Andreev reflection and the semiclassical Bogoliubov-de Gennes Hamiltonian: Resonant states

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ANDREEV REFLECTION AND THE SEMICLASSICAL BOGOLIUOBOV-DE GENNES HAMILTONIAN

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Abstract

We present a semi-classical analysis of the opening of superchannels in gated mesoscopic SNS or SFS junctions. For perfect Josephson junctions (i.e. hard-wall potential), this was considered by [2] in the framework of scattering matrices. Here we allow for imperfections in the junction, so that the complex order parameter continues as a smooth function, which is a constant in the superconducting banks, and vanishes rapidly inside the lead. The problem of finding quantization rules for Andreev states near energy E close to the Fermi level, reduces to finding the zeroes of the determinant of a monodromy matrix, which we characterize partially by means of geometric quantities.

1 Introduction.

Consider a narrow metallic lead, with a few transverse channels, connecting two superconducting contacts. For simplicity, the lead is identified with a 1-D structure, the interval $x \in [-L, L]$. The reference energy in the lead is taken as the Fermi level E_F, and the problem reduces to describing the dynamics of a quasi-particle (pair hole/electron) in the effective chemical potential $\mu(x) = E_F - E^{\perp}(x)$, where $E^{\perp}(x)$ denotes the transverse energy of the channel, obtained from adiabatic approximation. For simplicity, we shall consider only one transverse mode. Interaction with the superconducting bulk is modeled through the complex order parameter, or superconducting gap, $\Delta_0 e^{i\phi_\pm/2}$ at the boundary $\pm L$; due to the finite range of the junction, this interaction continues to a function $x \mapsto \Delta(x)e^{i\phi(x)/2}$, which vanishes rapidly inside the interval $[-L, L]$. For simplicity we will assume $\Delta(x)$ is smooth on $[-L, L]$, vanishes on $[-L', L']$, $0 < L' < L$ and $\phi(x) = \phi_\pm$ is a constant on $\pm x > 0$. We gauge the interaction with the supraconductor by setting $-\phi_- = \phi_+ = \phi$, so that $x \mapsto \phi(x)$ is odd, $\phi(x) = -\phi$ near $x = -L$ and $\phi(x) = \phi$ near $x = L$. Under these conditions, the dynamics of the quasi-particle is described by Bogoliubov-De Gennes Hamiltonian of the form

$$\mathcal{P}(x, \xi) = \begin{pmatrix} \xi^2 - \mu(x) & \Delta(x)e^{\frac{i}{2}\phi(x)} \\ \Delta(x)e^{-\frac{i}{2}\phi(x)} & -\xi^2 + \mu(x) \end{pmatrix} \qquad (1)$$

The energy surface $\Sigma_E = \{\det(\mathcal{P} - E) = \det(\mathcal{P} + E) = -(\xi^2 - \mu(x))^2 - \Delta(x)^2 + E^2 = 0\}$, foliated by two smooth lagrangian connected manifolds $\Lambda_E^\pm$, $\pm\xi > 0$ on $\Lambda_E^\pm$, is invariant under the reflections on the x and ξ axis. In this paper, we shall ignore tunneling between channels $\Lambda_E^\pm$, which is exponentially small, and focus on the upper branch Λ_E^+. Because of the smoothness of Δ, the exchange between holes and electrons occurs inside $[-L, L]$, we denote by $a = (x_0, \xi_0), a' = (-x_0, \xi_0) \in \Lambda_E^+$, the "branching points" defined by $\Delta(x_0) = E$ with $x_0 > 0$. We use throughout Weyl h-quantization $\mathcal{P}(x, hD_x)$ of Hamiltonian (1). So, if $\mathcal{I}$ denotes complex conjugation $\mathcal{I}u(x) = \overline{u(x)}$, i.e. $\mathcal{I}$ quantizes the reflection on the ξ axis, and $^\vee$ the reflection $^\vee u(x) = u(-x)$, we have PT symmetry

$$^\vee\mathcal{I}\mathcal{P}(x, hD_x) = \mathcal{P}(x, hD_x)\mathcal{I}^\vee \qquad (2)$$

and $\mathcal{P}(x, hD_x)$ is unitarily equivalent with the operator obtained by conjugation of charge (i.e. changing μ to $-\mu$) provided we take imaginary times (i.e. changing ξ to $i\xi$). Thus, such an hamiltonian has the CPT symmetry. For simplicity, we linearize the coefficients near x_0, i.e. we assume $\mu(x) = \text{Const}$ and $\Delta(x) = E + \alpha(x - x_0)$ near x_0, the slope $\alpha > 0$ will appear only as a rescaling of the "Planck constant" h which stands here for the characteristic wave-length of the quasi-particle relative to the size of the lead. This is what we call in the sequel the *Normal-Supraconductor (NS) junction model*. For the dynamics of the quasi-particle, the mechanism goes roughly as follows : An electron e^- moving in the metallic lead, say, to the right, with energy $0 < E \leq \Delta_0$ below the gap and kinetic energy $K_+(x) = \mu(x) + \sqrt{E^2 - \Delta(x)^2}$ is reflected back as a hole e^+ from the supraconductor, injecting a Cooper pair into the superconducting contact. The hole has kinetic energy $K_-(x) = \mu(x) - \sqrt{E^2 - \Delta(x)^2}$, and a momentum of the same sign as this of the electron, because of CPT symmetry. When $\inf_{[-L,L]} K_-(x) > 0$ it bounces along the lead to the left hand side and picks up a Cooper pair in the supraconductor, transforming again to the original electron state, a process known as Andreev reflection. Since $\mathcal{P}(x, hD_x)$ is self-adjoint, there is of course also an electron moving to the left, and a hole moving to the right (in fact, $\mathcal{P}(x, hD_x)$ is the hamiltonian for 2 pairs of quasi-particles), for no net transfer of charge can occur through the lead in absence of thermalisation. So we stress that Bogoliubov-de Gennes hamiltonian is only a simplified model for superconductivity, and a more thorough treatment should involve second quantization. Nevertheless, when $\phi \neq 0$, this process yields so called phase-sensitive Andreev states, carrying supercurrents proportional to the ϕ-derivative of the eigenenergies of $\mathcal{P}(x, hD_x)$. Note that $E > -\mu(x)$ is a "scattering energy" for the diagonal hamiltonian $\xi^2 - \mu(x)$, so the dynamics is more complicated than this of a particle in a potential well ; in some respect, the "barrier" $\Delta(x)$ is "transparent" to the pair hole/electron, which makes possible the exchange with Cooper pairs inside the supraconducting bulk. In the context of a perfect junction, the problem was handled in the formalism of scattering matrix and eigenvalue equation for the Andreev levels $E_n(h)$ was derived by matching the wave-functions and their derivatives at the NS junction [2]. It is of the form

$$\cos\phi = \cos(2\nu_0 E_n(h) - 2\arccos(\frac{E_n(h)}{\Delta_0})) \tag{3}$$

where $\nu_0 = \frac{L}{hv_F}$ (v_F is the Fermi velocity). This formula was generalized in the cas of a FS junction in [1]. In the semiclassical framework we should expect instead [5] (Sect 6) that the quantization condition takes the form

$$f_0(E_n(h)) + hf_1(E_n(h)) = (n + \frac{1}{2})h + \mathcal{O}(h^2) \tag{4}$$

where $f_0(E)$ is some action integral over a connected component (or cycle) of the energy surface , and $f_1(E)$ the measure over this cycle of some subprincipal symbol, with respect to Leray measure. We content in this report to characterize Andreev levels $E_n(h)$ by saying that the determinant of the monodromy matrix, relative to the complex vector bundle of a connection among microlocal solutions of $(\mathcal{P} - E)U = 0$ should vanish precisely when $E = E_n(h)$. We point out that our construction readily extend to the case of SFS junctions [1], by changing the energy level E by a quantity $\pm E_{\text{ex}}$, where E_{ex} denotes the exchange splitting energy.

2 A connection among microlocal solutions.

In the sequel we shall construct various microlocal solutions to $(\mathcal{P} - E)U(x, h) = 0$. Due to PT symmetry, we expect that when $E = E_n(h)$ is an eigenvalue, the solutions computed near a and extended up to a' would match with those computed near a'. In other words, the way of transporting a basis of the 2-D complex vector bundle of microlocal solutions determines a connnection, and we want to express the holonomy associated with this connection, still ignoring the coupling with $\xi < 0$. The quantization condition precisely means that we can select a global section among microlocal solutions. To describe the analytical setting, it is convenient to introduce the :

Définition 2.1 *We say $I(S, \varphi; \Xi)(x, h)$ is an admissible $\mathbf{C}^2$-valued lagrangian distribution if*

$$I(S, \varphi; \Xi)(x, h) = (2\pi h)^{-d/2} \int_{\mathbf{R}^d} e^{i\varphi(x,\Theta,\Xi,h)/h} S(x, \Theta, \Xi; h) d\Theta$$

Here Ξ is a vector-valued parameter, $\varphi(x, \Theta, \Xi, h)$ a non degenerate phase-function, and $S(x, \Theta, \Xi; h) = S_0(x, \Theta, \Xi; h) + hS_1(x, \Theta, \Xi; h) + \cdots$ a $\mathbf{C}^2$-valued amplitude (i.e. a classical symbol in h), $S_0 = \binom{e^{i\phi/2}X}{Y}$ possibly depending on h (with the property that $\phi(x) = \pm\phi$ is a constant on $\pm x > 0$). The symbols $X = X(x, \Theta, \Xi, h), Y = Y(x, \Theta, \Xi, h)$ have their principal part $\binom{X_0}{Y_0} = \lambda(x, \Theta, \Xi; h)\binom{X_0'}{Y_0'}$ proportional to a real vector $\binom{X_0'}{Y_0'} = \binom{X_0'}{Y_0'}(x, \Theta, \Xi, h)$. Again, $\lambda(x, \Theta, \Xi; h) \in \mathbf{C}$ can depend on h.

Here, all functions here are only defined microlocally. In general, microlocal solutions for $(\mathcal{P} - E)U(x, h) = 0$ will be obtained as linear combinations of such lagrangian distributions, with complex coefficients.

2.1 WKB solutions.

Most elementary admissible $\mathbf{C}^2$-valued lagrangian distributions, in the microlocal kernel of $(\mathcal{P} - E)$, are WKB solutions, obtained away from branching points. We diagonalize $\mathcal{P} - E$ outside the "branching points". The eigenvalues of $(\mathcal{P} - E)(x, \xi)$ are denoted by λ^I, and λ^{II}, so that the energy surface takes the form $\Sigma_E = \{\lambda^I = 0\}$ for $E > 0$. Thus $(\lambda^I)^{-1}(0) \cap \{\xi > 0\}$ is the union of 2 pieces of null bicharaceristics and join analytically at a' and a, as a connected component of $\det(\mathcal{P} - E) = 0$, and similarly for $(\lambda^I)^{-1}(0) \cap \{\xi < 0\}$. Again, for simplicity, we shall restrict to $\xi > 0$. Call the vector space of $\mathbf{C}^2$ generated by $\binom{1}{0}$ the space of (pure) *electronic states* and this by $\binom{0}{1}$ the space of (pure) *hole states*. Choose $(x_1, \xi_1) \in \Sigma_E \cap \{\xi > 0\}$ not a branching point, so that (x_1, ξ_1) belongs to an electronic state, or to a hole state. These states mix up when $\Delta(x) \neq 0$, but we can still sort them out semiclassically, outside (x_0, ξ_0). Then there is a unitary, hermitian matrix with smooth coefficients, $\mathcal{A}(x, \xi)$, defined along the piece $\rho = \rho_\pm \subset \{\xi > 0\}$ of Σ_E containing (x_1, ξ_1), and up to the branching points, such that

$$\mathcal{A}^*(\mathcal{P} - E)\mathcal{A} = \begin{pmatrix} \lambda^I & 0 \\ 0 & \lambda^{II} \end{pmatrix}$$

When $\Delta(x) \neq 0$ the normalized eigenvectors $(e^I(x, \xi), e^{II}(x, \xi))$ of $\mathcal{A}$ corresponding to eigenvalues $(\lambda^I, \lambda^{II})$ depend smoothly on (x, ξ), and can be extended throughout $x \in [-L, L]$ as a smooth section valued in the circle. Moreover, each eigenvector can be multiplied by a phase factor $\exp i\omega(x,\xi)$, allowing for monodromy in the fibre bundle of WKB solutions. When $E > 0$, we are only interested in the eigenvector $e = e^I$ belonging to $\lambda^I = 0$.

It is possible to implement this diagonalization at the level of operators, and we recall that the first 2 terms of the Weyl symbol of $\lambda^I(x, hD_x, h)$ are computed in [5] (Sect 6). It is convenient to keep the (real valued) subprincipal symbol $\lambda^I_1(x,\xi)$ together with the principal symbol $\lambda^I_0(x,\xi)$, so let

$$\widehat{\lambda}^I(x,\xi,h) = \lambda^I_0(x,\xi) + h\lambda^I_1(x,\xi)$$

We look for a WKB solution $\widetilde{U}(x,h)$ of $\mathcal{A}^*(\mathcal{P}-E)\mathcal{A}\widetilde{U}(x,h) = 0$, and take $\widetilde{U}(x,h) = e^{i\varphi^I(x,h)/h}(u(x,h),0)$ where φ^I solves the modified eikonal equation $\widehat{\lambda}^I(x,\partial_x\varphi^I,h) = 0$, and the symbol $u = u_0 + hu_1 + \cdots$ is uniquely determined up to a constant factor by solving transport equations along ρ. In particular $u_0(x,h)$ satisfies :

$$\partial_\xi\widehat{\lambda}^I(x,\partial_x\varphi^I,h)\partial_x u_0 + \frac{1}{2}\frac{\partial^2}{\partial x\partial\xi}\widehat{\lambda}^I(x,\partial_x\varphi^I,h)u_0 = 0$$

so u_0 can be chosen to be real. Applying $\mathcal{A}$ we get

$$U(x,h) = \mathcal{A}\tilde{U}(x,h) = e^{\frac{i}{h}\varphi_1(x,h)}(u_0(x,h)\mathrm{e}(x,\partial_x\varphi^I) + \mathcal{O}(h))$$

This way, we have constructed an admissible $\mathbf{C}^2$-valued lagrangian distribution $U(x,h)$, such that $(\mathcal{P}-E)U(x,h) = 0$ microlocally near (the interior of) ρ. In particular, the space of microlocal solutions U of $\lambda^I(x,hD_x,h;E)U = 0$ supported in $\xi > 0$ is of dimension 2.

2.2 Microlocal solutions for the NS junction model.

Close to the branching points, we consider now more complicated admissible $\mathbf{C}^2$-valued lagrangian distributions. Near $a = (x_0,\xi_0)$, the NS junction model Hamiltonian, in h-Fourier representation, takes the form $\mathcal{P}^a(-hD_\xi,\xi) =$

$$\begin{pmatrix} \xi^2-\mu & e^{\frac{i}{2}\phi}(E-\alpha(hD_\xi+x_0)) \\ e^{-\frac{i}{2}\phi}(E-\alpha(hD_\xi+x_0)) & -\xi^2+\mu \end{pmatrix}$$

where $\mu = \xi_0^2$ is a constant. Consider the eigenvalue equation $(\mathcal{P}^a(-hD_\xi,\xi)-E)U = 0$, where $U = \begin{pmatrix}\widehat{\varphi}_1 \\ \widehat{\varphi}_2\end{pmatrix}$.
Clearly, the system decouples, and to account for time-reversal symmetry, it is convenient to introduce the scaling parameter $\beta = \sqrt{\alpha}(2\xi_0)^{-3/2}$, together with the changes of variables $\xi = \xi_0(\pm 2\beta\xi' + 1)$. The functions $\widetilde{u}_{\pm\beta}(\xi') = (\xi^2-\mu-E)^{-1/2}e^{-i(E-\alpha x_0)\xi/\alpha h}\widehat{\varphi}_2$ satisfy a second order ODE of the form

$$(\tilde{P}_{\pm\beta}(-hD_{\xi'},\xi',h) - \frac{E_1^2}{\beta^2})\tilde{u}_{\pm\beta}(\xi') = 0 \tag{5}$$

with $E_1 = (2\xi_0)^{-2}E$, and

$$\begin{aligned}\tilde{P}_{\pm\beta}\ (-hD_{\xi'},\xi',h) &= (hD_{\xi'})^2 + (\xi' \pm \beta\xi'^2)^2 \\ &+ (2\xi_0\beta h)^2\,\frac{(2\beta^2\xi'^2 \pm 2\beta\xi' + \frac{3}{4} + E_1)}{(\beta^2\xi'^2 + \beta\xi' - E_1)^2}\end{aligned} \tag{6}$$

Viewed as a h-PDO's of order 0, micrlocally defined near $(x',\xi') = 0$, $\tilde{P} = \tilde{P}_{\pm\beta}$ can be taken to the normal form of a harmonic oscillator. More precisely, there exists a real-valued analytic symbol $F(t,h) = F_{\pm\beta}(t,h) \sim \sum_{j=0}^{\infty} F_j(t)h^j$, defined for $t \in \mathrm{neigh}(0)$, $F_0(0) = 0$, $F_0'(0) = \frac{1}{2}$, $F_1(t) = \mathrm{Const}$, and (formally) unitary FIO's $A = A_{\pm\beta}$ whose canonical transformations κ_A defined in a neighborhood of (0,0), are close to identity and map this point onto itself, such that

$$A^*F(\tilde{P},h)A = P_0 = \frac{1}{2}((hD_\eta)^2 + \eta^2 - h)$$

From the point of vue of pseudo-differential calculus, it is important to modify the canonical relation κ_A by a term $\mathcal{O}(h)$ in order to improve Egorov theorem by an accuracy $\mathcal{O}(h^2)$. In our problem this phase shift will be responsible for monodromy. Define the large parameter ν by $F(\frac{E^2}{2\xi_0\alpha},h) = \nu h$. So $\tilde{u} = \tilde{u}_{\pm\beta}$ solves (5) microlocally near (0,0) iff $v = A^*\tilde{u}$ solves Weber equation $(P_0-\nu h)v = 0$ microlocally near (0,0), when $\nu h \sim \frac{E^2}{4\xi_0\alpha}$ is small enough. The well known parabolic cylinder functions D_ν and $D_{-\nu-1}$, whose integral representation is the inverse Laplace transform

$$D_\nu(\zeta) = \frac{\Gamma(\nu+1)}{2i\pi}e^{-\zeta^2/4}\int_\infty^{(0^+)} e^{-\zeta s - s^2/2}(-s)^{-\nu}\frac{ds}{s}$$

form a basis of solutions of $\frac{1}{2}((hD_\eta)^2 + \eta^2 - h)v = \nu v$. Let us write

$$v = \sum_{\epsilon=\pm 1}\alpha_\epsilon^{(\nu)}D_\nu(\epsilon(h/2)^{-1/2}\cdot) = \sum_{\epsilon=\pm 1}\alpha_\epsilon^{(-\nu-1)}D_{-\nu-1}(i\epsilon(h/2)^{-1/2}\cdot) \tag{7}$$

for complex constants $\alpha_\epsilon^{(\nu)}$, $\alpha_\epsilon^{(-\nu-1)}$. To distinguish between $\pm\beta$, we index also the constants $\alpha_\epsilon^{(\nu)}$ by $\pm\beta$. We call $h' = \alpha h$ the new "Planck constant". By a careful analysis involving the search for critical points of the phase functions, and stationary phase expansions, we obtain :

Proposition 2.1 *For $x < x_0$ near x_0, there are 2 basis of oscillating microlocal solutions of $(\mathcal{P}^a - E)U = 0$ indexed by $\epsilon = \pm 1$:*

$$\sum_\rho U^{a,\nu}_{\rho,\epsilon,\pm\beta}(x,h'), \quad \sum_\rho U^{a,-\nu-1}_{\rho,\epsilon,\pm\beta}(x,h')$$

which satisfy :

$$U^{a,\nu}_{-,\epsilon,\beta} = U^{a,\nu}_{+,\epsilon,-\beta}, \quad U^{a,-\nu-1}_{-,\epsilon,\beta} = U^{a,-\nu-1}_{+,\epsilon,-\beta}$$

Recall that the branch with $\rho = \rho_\pm = \pm 1$ is microlocalized on $\rho_\pm$; the part on ρ_+ ($\xi > \xi_0$ near a), belongs to the electron state, while the part ρ_- ($\xi < \xi_0$ near a) belongs to the hole state. Each of these solutions is an admissible $\mathbf{C}^2$-valued lagrangian distribution in the sense of Definition 1.1. Divide all microlocal solutions by the trivial factor $e^{i\pi/4}e^{iE_0\xi_0/h'}$, $E_0 = E - \alpha x_0$. Then with the notations of (7) the general solution of $(\mathcal{P}^a - E)U = 0$ is of the form

$$U = \sum_{\rho,\epsilon}\alpha^{(\nu)}_{\epsilon,\pm\beta}U^{a,\nu}_{\rho,\epsilon,\pm\beta} = \sum_{\rho,\epsilon}\alpha^{(-\nu-1)}_{\epsilon,\pm\beta}U^{a,-\nu-1}_{\rho,\epsilon,\pm\beta}$$

Consider similarly the solutions near a'. We have :

$$U^{a',\nu}_{\rho,\epsilon,-\beta} = {}^\vee\mathcal{I}U^{a,\nu}_{\rho,\epsilon,\beta}, \quad U^{a',-\nu-1}_{\rho,\epsilon,-\beta} = {}^\vee\mathcal{I}U^{a,-\nu-1}_{\rho,\epsilon,\beta}.$$

Note that the functions $U^{(\nu)}_{\rho,\epsilon,\pm\beta}$ and $U^{(-\nu-1)}_{\rho,\epsilon,\pm\beta}$ differ essentially by $\mathcal{O}(h)$ in their phase functions. The sum over $\rho = \pm 1$ is due to the contributions to stationary phase, for a given x, of the critical points on $\rho_\pm$. Note also that in this region where μ is a constant, $U_{\rho,\epsilon,\pm\beta} = e^{\frac{i}{h}x\xi_0}\mathcal{U}_{\rho,\epsilon,\pm\beta;h'}$ with $\mathcal{U}_{\rho,\epsilon,\pm\beta;h'}$ oscillating on a frequency scale $\frac{1}{h'} = \frac{1}{\alpha h}$, so if we think of the slope α to be large, $U_{\rho,\epsilon,\pm\beta}$ behaves as a plane wave $e^{\frac{i}{h}x\xi_0}$, modulo a slow varying function.

2.3 The monodromy matrix.

From now on we just keep the second basis $D_{-\nu-1}(i\epsilon\zeta)$ (to fix the ideas) of solutions of Weber equation, $D_\nu(\epsilon\zeta)$ being useful only if we consider $x > x_0$ and the coupling with $\xi < 0$. We sum over $\rho = \pm 1$ the branches of microlocal solutions defined above, and set $U^{a,-\nu-1}_{\epsilon,\beta} = \sum_\rho U^{a,-\nu-1}_{\rho,\epsilon,\beta}$, and similarly for a'. We can uniquely extend from a, as WKB solutions, the microlocal solutions $U^a = U^{a,-\nu-1}_{\epsilon,\beta}$ along $\rho_\pm$ towards a'. Similarly we can construct corresponding microlocal solutions $U^{a'}$ in the neighborhood of a', and extend them along $\rho_\pm$ towards a. Denote for short by α_1, α_2 the coefficients $\alpha^{(-\nu-1)}_{\epsilon,\pm}$, etc.... Because of symmetry (2) and Proposition 2.1, the extension along $\rho_\pm$ of the linear combination $\alpha_1 U^{a,-\nu-1}_{+,\beta} + \alpha_2 U^{a,-\nu-1}_{-,\beta}$ will be a linear combination $\beta_1 U^{a',-\nu-1}_{+,-\beta} + \beta_2 U^{a',-\nu-1}_{-,-\beta}$ and the coefficients $\binom{\beta_1}{\beta_2}$ are related to $\binom{\alpha_1}{\alpha_2}$ by

$$\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix} = M^{a,a'}\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} \tag{8}$$

where $M^{a,a'} = \begin{pmatrix} d_{11} & d_{12}\\ d_{21} & d_{22}\end{pmatrix} \in U(2)$. This is the monodromy matrix. Similarly, we obtain $M^{a',a}$ by extending from the left to the right, and due to symmetry, $M^{a',a} = (M^{a,a'})^{-1} = (M^{a,a'})^*$. Moreover we have $|d_{11}| = |d_{22}|$, $|d_{12}| = |d_{21}|$, so that if $\Delta_{ij} = \arg d_{ij}$, the unitarity relation takes the form $\Delta_{11} + \Delta_{22} = \Delta_{12} + \Delta_{21} \pm \pi$ and $|d_{11}|^2 + |d_{21}|^2 = 1$, while $\det M^{a,a'} = e^{i(\Delta_{12}+\Delta_{21})}$.

Using the WKB solutions of Sect 2.1, and conservation laws resulting from the fact that the Wronskian for solutions of the differential operator (6) is a constant, we can in particular compute the trace of $M^{a,a'}$ in term of the action integral $S_+ = \int_{-x_0}^{x_0}\xi_+(x,h)dx = 2\int_0^{x_0}\xi(x,h)dx$, where $\widehat{\lambda}^I(x,\xi_+(x,h),h) = 0$. Namely, modulo an inessential factor,

$$\mathrm{Tr}M^{a,a'} = d_{11} + d_{22} \sim e^{\frac{i}{h}S_+}e^{-\frac{i}{4}\phi}\cos(\pi\nu + \frac{\phi}{4}) \tag{9}$$

3 The normalized microlocal solutions and the approximate Bohr-Sommerfeld quantization rule.

Following a classical procedure in Fredholm theory, we can translate the original eigenvalue problem for $\mathcal{P}$ into a finite dimensional problem via the Grusin operator [6](Sect 4), but due to the fact that we have ignored coupling with the bicharacteristics in the lower half-plane $\xi < 0$, the "simplified" Grusin problem is not well-posed. So we proceed a little formally taking only in account the microlocal kernel K_0 of $\mathcal{P} - E$ in $(x,\xi) \in]-x_0, x_0[\times R_+$. First we normalize the basis in K_0, obtained in Proposition 1.2, using generalized wronskians introduced in ([4],[5],[6]) and adapted to a system of h-PDO's in [7]. Namely, let $\chi = \chi^a$ be a cut-off supported on a domain containing (the interior of) $\rho_+ \cup \rho_-$, equal to 1 near a, and to 0 near a', $\omega = \omega^a$ be a small neighborhood of $(\rho_+ \cup \rho_-) \cap \mathrm{supp}[\mathcal{P}, U]$, and χ_ω be a cut-off equal to 1 near ω. If U, V are such solutions, we call

$$\mathcal{W}(U,\overline{V}) = (\chi_\omega \frac{i}{h}[\widetilde{\mathcal{P}},\chi]U|V)$$

the *microlocal wronskian* of $(U,\overline{V})$ in ω. This quantity is independent, modulo error terms $\mathcal{O}(h^\infty)$ of the choices of χ and χ_ω as above. For each of the U's above, $\mathcal{W}(U,\overline{U})$ is a (positive) classical symbol, allowing to normalize U so that $\mathcal{W}(U,\overline{U}) = 2$. We shall denote the normalized solutions by the same letter. Consider also

$$F^{a,-\nu-1}_{\epsilon,\beta} = \chi_{\omega^a}\frac{i}{h}[\mathcal{P},\chi^a]U^{(a,-\nu-1)}_{\epsilon,\beta}$$

and similarly $F^{a',-\nu-1}_{\epsilon,-\beta}$, which span the microlocal co-kernel K_0^* of $\mathcal{P} - E$ in $]-x_0, x_0[\times\mathbf{R}_+$, as $\epsilon = \pm 1$. For $\epsilon = 1$, let U_1 be equal to $U_1^a = U^{a,-\nu-1}_{+,\beta}$ near a, and to

$$U_1^{a'} = (1-\chi^{a'})U^{a,-\nu-1}_{+,\beta,\mathrm{ext}} = (1-\chi^{a'})(d_{11}U^{a',-\nu-1}_{+,-\beta} + d_{21}U^{a',-\nu-1}_{-,-\beta})$$

near a'. We compute the scalar products $R_+U_1 =$

$$((U_1^a|F^{a,-\nu-1}_{+,\beta}), (U_1^a|F^{a,-\nu-1}_{-,\beta}), (U_1^{a'}|F^{a',-\nu-1}_{+,-\beta}), (U_1^{a'}|F^{a',-\nu-1}_{-,-\beta}))$$

using microlocal Wronskians. Consider the classical symbols

$$c^a_{\pm,\mp} = (U^{a',-\nu-1}_{\pm,-\beta}|F^{a',-\nu-1}_{\mp,-\beta}), \gamma^{a'}_\epsilon = Im(\chi^{a'}U^{a',-\nu-1}_{\epsilon,-\beta}|F^{a',-\nu-1}_{\epsilon,-\beta}),$$

and $\delta^{a'}_{\pm,\mp} = ((1-\chi^{a'})U^{a',-\nu-1}_{\pm,-\beta}|F^{a',-\nu-1}_{\mp,-\beta})$, which can be evaluated explicitely using Proposition 2.1 and stationary phase expansions, as in [7](Lemma 7.2). We define similarly U_2 for $\epsilon = -1$, and also with similar notations, U_3, U_4 by moving from a' towards a instead, so we find

$$R_+U_1 = (2,\ c^a_{+,-},\ d_{11}(1-i\gamma^{a'}_+) + d_{21}\delta^{a'}_{-,+},\ d_{11}\delta^{a'}_{+,-} + d_{21}(1-i\gamma^{a'}_-))$$

$$R_+U_2 = (c^a_{-,+},\ 2,\ d_{12}(1-i\gamma^{a'}_+) + d_{22}\delta^{a'}_{-,+},\ d_{12}\delta^{a'}_{+,-} + d_{22}(1-i\gamma^{a'}_-))$$

$$R_+U_3 = (e_{11}(1-i\gamma^a_+) + e_{21}\delta^a_{-,+},\ e_{11}\delta^a_{+,-} + e_{21}(1-i\gamma^a_-),\ 2,\ c^{a'}_{+,-})$$

$$R_+U_4 = \big(e_{12}(1-i\gamma^a_+) + e_{22}\delta^a_{-,+},\ e_{12}\delta^a_{+,-} + e_{22}(1-i\gamma^a_-),\ c^{a'}_{-,+}, 2\big)$$

Consider now the matrix G consisting of the columns R_+U_j, $1 \le j \le 4$. This is the Gram matrix of the vectors U_j in the basis $(F^{a,-\nu-1}_{\epsilon,\beta}, F^{a',-\nu-1}_{\epsilon,-\beta})_{\epsilon=\pm 1}$. We can show that, modulo $\mathcal{O}(h^\infty)$, the relations

$$c^a_{-,+} = \overline{c^a_{+,-}},\ |\delta^{a'}_{+,-}| = |\delta^a_{+,-}|,\ |\delta^{a'}_{-,+}| = |\delta^a_{-,+}|,$$
$$\gamma^{a'}_{-} + \gamma^a_{-} = \gamma^{a'}_{+} + \gamma^a_{+} = 0$$

hold, which make of G an hermitean matrix. It follows that its spectrum is real, with a possible degeneracy, so are the functions defining the branches for the equation $\det G(E,h) = 0$.

Proposition 3.1 *The vectors U_j are colinear, precisely when E satisfies $\det G(E,h) = 0$, which is an equation with real coefficients. This means there exists for these values of E a smooth section U solving $(\mathcal{P} - E)U = 0$, globally on $]-x_0, x_0[\times \mathbf{R}_+$.*

Of course, relation (8) is not sufficient for computing $M^{a,a'}$, and getting an explicit form for the Bohr-Sommerfeld rule in term of ϕ, but further information can still be extracted by considering the vector-bundle associated with a basis of eigenvectors $e^I_\pm$ of $\mathcal{P}$ (see [5]). A more thorough spectral analysis should also involve a microlocal insight into the junction, e.g. $x > x_0$. This relies on the "infinitesimal" invariance by conjugation of charge : namely, we can change β into $\pm i\beta$, without altering equation (5), and more generally, consider the family of distributions, obtained by extending $\widetilde{u}_\beta(\xi')$, say, along a path $e^{i\gamma}\beta$, $0 \leq \gamma \leq 2\pi$ in the complex domain (see also [3] for related topics). Note also that $P_{\pm\beta}(-hD_\xi, \xi, h)$ is *not* microhyperbolic at (x_0, ξ_0) in the directions $(0, \pm id\xi)$, see e.g. [5] (Sect 10). The germ of corresponding microlocal solutions in $x > x_0$ have complex phases, not simply purely imaginary as in usual tunneling problems for Schrödinger operators.

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